FREE-ENERGY BASED POTENTIALS FOR MULTISCALE SIMULATIONS SOFT MATTER

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I will discuss two recently introduced systematic coarse-graining methods that provide transferable coarse-grained potentials for scale-bridging simulations of soft matter systems.

The first method is based on direct calculation of pair potentials in the gas or liquid phase with thermodynamic integration or free energy perturbation methods. These so-called Conditional Reversible Work (**CRW**) potentials have been calculated for aliphatic groups, which serve as coarse-grained building blocks in macromolecular systems. It will be show that CRW models are chemically transferable to coarse-grained linear alkanes and thermodynamically transferable in the liquid phase branch of the phase diagram (1 atm.) between the melting and boiling points.

The second method is an extension of iterative Boltzmann inversion (IBI) and reproduces the density fluctuations at small scales which determine the thermodynamic solvation properties of multicomponent solutions. This so-called Kirkwood-Buff-IBI (**KB-IBI**) method has been applied to develop single-site solvent models for aqueous solutions of urea and methanol and was used to study salting-in of hydrophobic solutes and the peptide group by urea.

CRW and KB-IBI models exhibit promising chemical and thermodynamic transferability and may potentially be applied to study phenomena away from equilibrium on mesoscopic time and length scales.